

09/759,633

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09/759,633

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FILE 'HOME' ENTERED AT 11:59:35 ON 18 MAR 2004

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STRUCTURE FILE UPDATES: 17 MAR 2004 HIGHEST RN 664302-53-8
DICTIONARY FILE UPDATES: 17 MAR 2004 HIGHEST RN 664302-53-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
Uploading C:\STNEXP4\QUERIES\09759633.str

L1 STRUCTURE UPLOADED

```
=> s 11 ful
FULL SEARCH INITIATED 12:00:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      407 TO ITERATE
```

100.0% PROCESSED 407 ITERATIONS 25 ANSWERS
SEARCH TIME: 00.00.01

L2 25 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE
ENTRY
TOTAL
SESSION
155.42
155.63

09/759,633

FILE 'CAPLUS' ENTERED AT 12:00:12 ON 18 MAR 2004
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FILE COVERS 1907 - 18 Mar 2004 VOL 140 ISS 12
FILE LAST UPDATED: 17 Mar 2004 (20040317/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12
L3 10 L2

=> d 13 ibib hitstr abs 1-10

L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:526050 CAPLUS
DOCUMENT NUMBER: 135:107149
TITLE: Synthesis, antibacterial activity and RNA polymerase inhibition of phenylamidine derivs.
INVENTOR(S): Li, Leping; Chen, Xiaoqui; Fan, Pingchen; Mihalic, Jeffrey Thomas; Cutler, Serena
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001051456	A2	20010719	WO 2001-US1219	20010112
WO 2001051456	A3	20011220		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002045749	A1	20020418	US 2001-759633	20010112
EP 1246795	A2	20021009	EP 2001-914329	20010112
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,			

09/759,633

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2003519676 T2 20030624 JP 2001-551838 20010112
PRIORITY APPLN. INFO.: US 2000-175892P P 20000113
WO 2001-US1219 W 20010112

OTHER SOURCE(S): MARPAT 135:107149

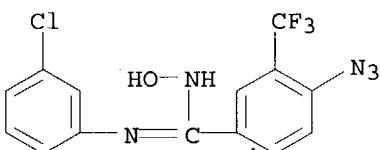
IT 350486-82-7P 350486-84-9P 350486-86-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(synthesis, antibacterial activity and RNA polymerase inhibition of phenyl- and heterocyclhydroxyamidine derivs.)

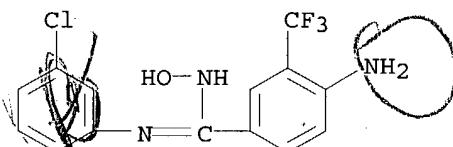
RN 350486-82-7 CAPLUS

CN Benzenecarboximidamide, 4-azido-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



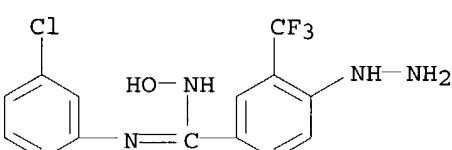
RN 350486-84-9 CAPLUS

CN Benzenecarboximidamide, 4-amino-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350486-86-1 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-hydrazino-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 350487-08-0P 350487-09-1P 350487-13-7P
350487-14-8P 350487-15-9P 350487-18-2P
350487-19-3P 350487-20-6P 350487-22-8P
350487-25-1P 350487-26-2P 350487-31-9P
350487-96-6P 350487-97-7P 350487-98-8P
350487-99-9P

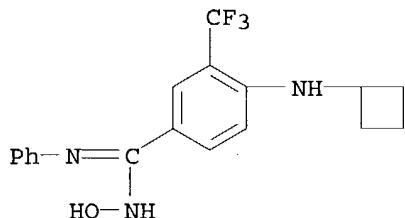
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

09/759, 633

BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis, antibacterial activity and RNA polymerase inhibition of
phenyl- and heterocyclhydroxyamidine derivs.)

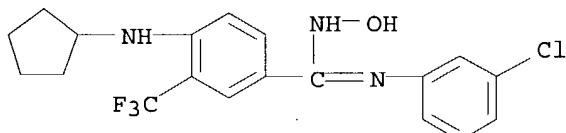
RN 350487-08-0 CAPLUS

CN Benzenecarboximidamide, 4-(cyclobutylamino)-N-hydroxy-N'-phenyl-3-
(trifluoromethyl)- (9CI) (CA INDEX NAME)



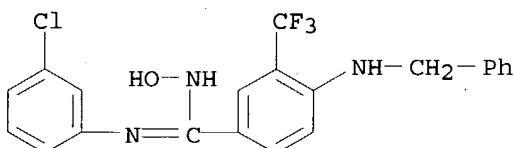
RN 350487-09-1 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-(cyclopentylamino)-N'-hydroxy-
3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



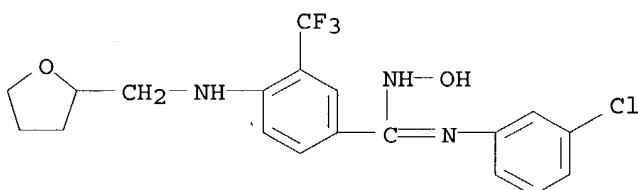
RN 350487-13-7 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-
[(phenylmethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-14-8 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(tetrahydro-2-
furanyl)methyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

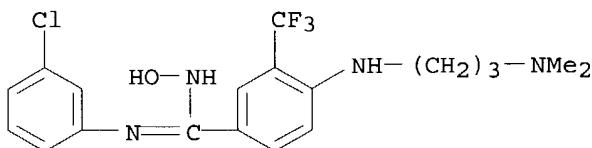


RN 350487-15-9 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-[(3-

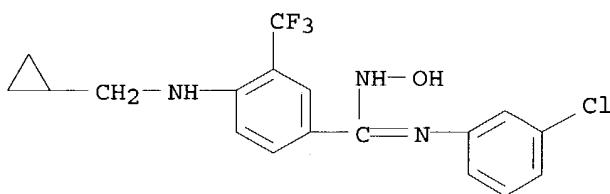
09/759, 633

(dimethylamino)propyl]amino]-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



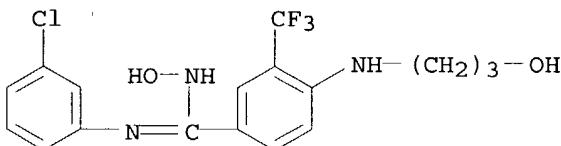
RN 350487-18-2 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-[(cyclopropylmethyl)amino]-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



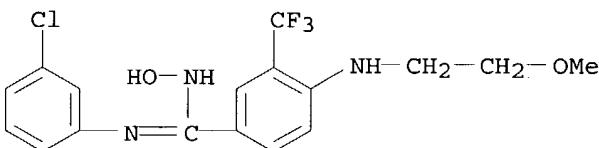
RN 350487-19-3 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(3-hydroxypropyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-20-6 CAPLUS

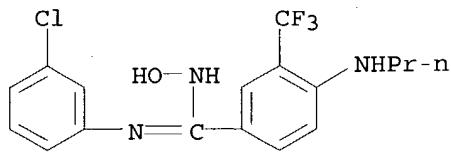
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(2-methoxyethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



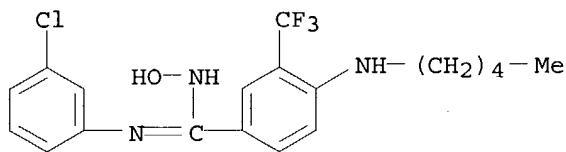
RN 350487-22-8 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(propylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

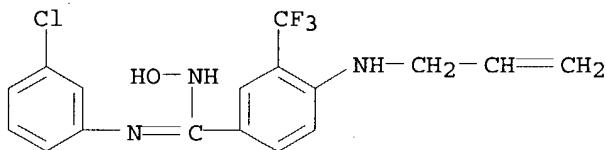
09/759, 633



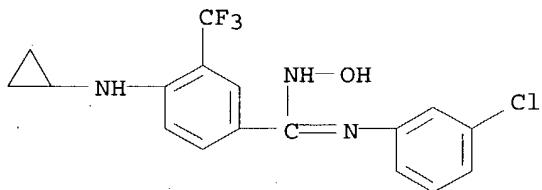
RN 350487-25-1 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(pentylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



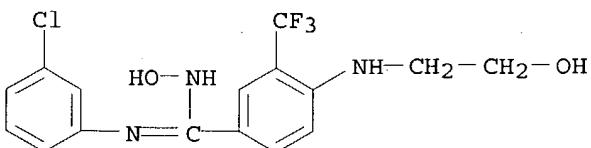
RN 350487-26-2 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(2-propenylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-31-9 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-(cyclopropylamino)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



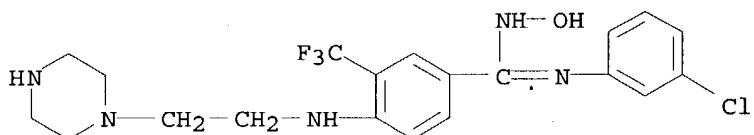
RN 350487-96-6 CAPLUS
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(2-hydroxyethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



09/759,633

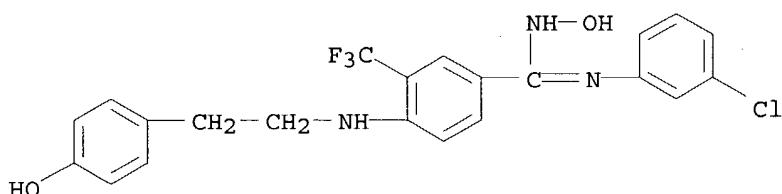
RN 350487-97-7 CAPLUS

CN Benzenecarboximidamide, N- (3-chlorophenyl)-N'-hydroxy-4- [[2- (1-piperazinyl)ethyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



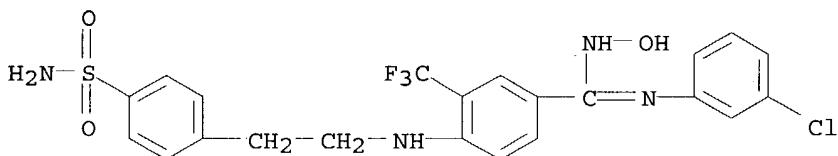
RN 350487-98-8 CAPLUS

CN Benzenecarboximidamide, N- (3-chlorophenyl)-N'-hydroxy-4- [[2- (4-hydroxyphenyl)ethyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

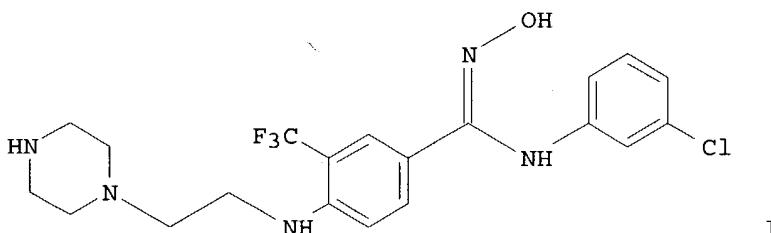


RN 350487-99-9 CAPLUS

CN Benzenecarboximidamide, 4- [[2- [4- (aminosulfonyl)phenyl]ethyl]amino]-N- (3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



GI

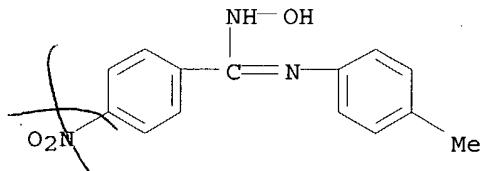


I

AB Synthesis of hydroxyamidines, e.g. (I) and related compds. are disclosed which are suitable as antibacterial agents by their inhibition of RNA polymerase. Antibacterial activity against *S. aureus* and *E. coli* are given.

09/759, 633

L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:276393 CAPLUS
DOCUMENT NUMBER: 133:73985
TITLE: A convenient synthesis of 3,4-disubstituted-1,2,4-thiadiazole-5(4H)-thiones
AUTHOR(S): Agirbas, Hikmet; Kahraman, Kazim
CORPORATE SOURCE: Department of Chemistry, Kocaeli University, Izmit, 41300, Turk.
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1998), 134/135, 381-389
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 2630-07-1, N-Hydroxy-N'-(4-methylphenyl)-4-nitrobenzenecarboximidamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiadiazolethiones by rearrangement of oxadiazolethione intermediates)
RN 2630-07-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-N'-(4-methylphenyl)-4-nitro- (9CI) (CA INDEX NAME)



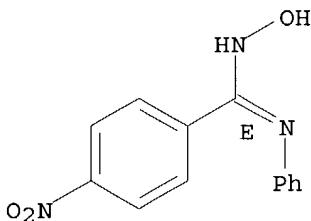
AB 3,4-Disubstituted-1,2,4-oxadiazole-5(4H)-ones were obtained from the reaction of substituted amide oximes with Et chloroformate. These compds. were treated with P2S5 to give corresponding 1,2,4-oxadiazole-5-thiones. Rearrangement of 1,2,4-oxadiazole-5-thiones, catalyzed by metallic copper, yielded 1,2,4-thiadiazole-5-ones. The reaction of 1,2,4-thiadiazole-5-ones with P2S5 gave 1,2,4-thiadiazole-5-thiones.
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:908286 CAPLUS
DOCUMENT NUMBER: 124:102365
TITLE: Crystal and molecular structure of N-phenyl-4-nitrobenzamidoxime
AUTHOR(S): Buzykin, B. I.; Dokuchaev, A. S.; Kharitonova, O. A.
CORPORATE SOURCE: A. E. Arbuzov Inst. Org. Phys. Chem., Russian Acad. Sci., Kazan, 420083, Russia
SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1995), (8), 1516-19
CODEN: IASKEA
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT 172540-77-1
RL: PRP (Properties)
(crystal structure of)
RN 172540-77-1 CAPLUS

09/759, 633

CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



AB An x-ray study of N-phenyl-4-nitrobenzamidoxime (1) was performed. Crystallog. data and atomic coordinates are given. Two crystallog. independent mols. have a planar Z-configuration of amidoxime with s-trans-conformation of these fragments related to =N-O and C-N(H) bonds. Intramol. NH...O bond is observed. Rotation angle of nitrophenyl and Ph rings related to amidoxime plane [ONCN] is -57 and -32° in 1A and -38 and -22° in 1B correspondingly. Rotation around C(1)-N(2) bond is -28 (1A) and -35° (1B). 1A and 1B mols. form oxime dimers in crystals due to two intermol. H-bond =N... (HO)', dimers forming double chains due to two more H-bonds NH... (O2N).

L3 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:128321 CAPLUS

DOCUMENT NUMBER: 116:128321

TITLE: Reaction of triethyl orthoformate with mono-substituted amidoximes

AUTHOR(S): Andrianov, V. G.; Eremeev, A. V.

CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1991), 27(8), 1604-7

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

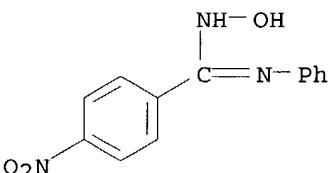
IT 57767-04-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with tri-Et orthoformate)

RN 57767-04-1 CAPLUS

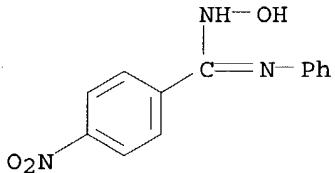
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)



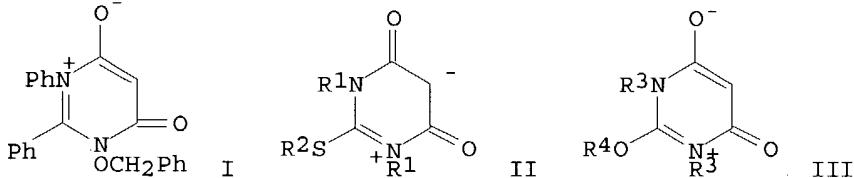
AB The reaction of 4-O2NC6H4C(:NOH)NHR (I; R = Me, Et, Ph) with CH(OEt)3 gave 4-O2NC6H4C(:NO2CNHR)NHR in 33-38% yield. I in turn were prepared from 4-O2NC6H4CCl:NOH and RNH2.

09/759,633

L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:62359 CAPLUS
DOCUMENT NUMBER: 88:62359
TITLE: Syntheses of heterocycles, CCVII. Mesoionic pyrimidines and thiazines
AUTHOR(S): Ziegler, Erich; Steiger, Wilfried; Strangas, Charilaos
CORPORATE SOURCE: Inst. Org. Chem., Univ. Graz, Graz, Austria
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1977), 32B(10), 1204-8
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: German
IT 57767-04-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbon suboxide)
RN 57767-04-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)



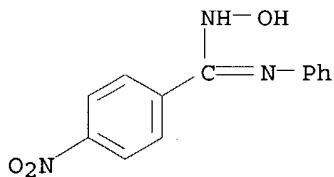
GI



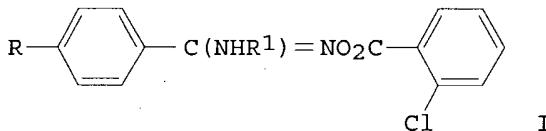
AB $\text{CH}_2(\text{CO}_2\text{N:CRNHPh})_2$ ($\text{R} = 4-\text{O}_2\text{NC}_6\text{H}_4, 3-\text{O}_2\text{NC}_6\text{H}_4, 2-\text{ClC}_6\text{H}_4$) were obtained by treating HON:CRNHPh with C_3O_2 . $\text{PhCH}_2\text{ON:CPhNHPh}$ similarly gave the pyrimidinone I. II ($\text{R}1 = \text{Ph}, 4-\text{MeC}_6\text{H}_4, 2-\text{MeC}_6\text{H}_4; \text{R}2 = \text{Me, Et}$) were similarly obtained from $\text{R}1\text{N:C(SR}2\text{)NHR}1$ and III ($\text{R}3 = \text{cyclohexyl, Ph, 4-MeC}_6\text{H}_4, \text{R}4 = \text{Me, Et}$) from $\text{R}3\text{NHC(OR}4\text{):NR}3$.

L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:542212 CAPLUS
DOCUMENT NUMBER: 85:142212
TITLE: Elimination reactions with anilide oxime
o-chlorobenzoates: rearrangement into carbodiimides
by reaction with sodium tert-amylate
AUTHOR(S): Garapon, Jacques; Sillion, Bernard
CORPORATE SOURCE: Inst. Fr. Pet., CEN, Grenoble, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1975),
(11-12, Pt. 2), 2671-6
CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal
 LANGUAGE: French
 OTHER SOURCE(S): CASREACT 85:142212
 IT 57767-04-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation of)
 RN 57767-04-1 CAPLUS
 CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX
 NAME)



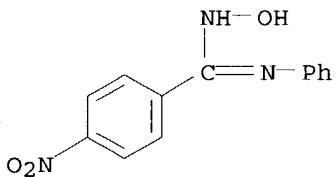
GI



AB The elimination reaction of I (R = H, p-MeO, p-NO₂; R₁ = Ph, cyclohexyl, 2,6-Me₂C₆H₃) with sodium tert-amylate occurred via a carbodiimide intermediate. A concerted reaction mechanism was postulated.

L3 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1975:592705 CAPLUS
 DOCUMENT NUMBER: 83:192705
 TITLE: Synthetic reactions using transition metal complexes.
 Conversion of amide oximes into amidines by
 pentacarbonyliron and evidence for imine intermediates
 in the deoximation of ketoximes
 AUTHOR(S): Dondoni, Alessandro; Barbaro, Gaetano
 CORPORATE SOURCE: Ist. Chim. Org., Univ. Bologna, Bologna, Italy
 SOURCE: Journal of the Chemical Society, Chemical
 Communications (1975), (18), 761-2
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 83:192705
 IT 57767-04-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reductive dehydroxylation of, by pentacarbonyliron)
 RN 57767-04-1 CAPLUS
 CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX
 NAME)

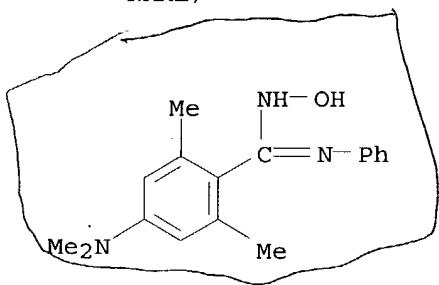
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AB Treatment of $RC(:NOH)NR_1R_2$ ($R = Ph$, $R_1 = H$, $R_2 = Ph$, C_6H_4Cl-p ; $R = Ph$, $R_1 = Me$, $R_2 = Ph$, Me ; $R = Mesityl$, $p-O_2NC_6H_4$, $R_1 = H$, $R_2 = Ph$) with ≥ 1 equiv $Fe(CO)_5$ in refluxing dry THF gave 70-90% $RC(:NH)NR_1R_2$. $2,4,6-Me_3C_6H_2C(:NOH)Me$ reacted similarly.

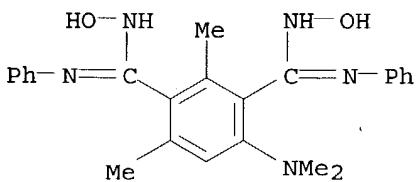
L3 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1967:454096 CAPLUS
DOCUMENT NUMBER: 67:54096
TITLE: Nitrile oxides. IX. Basic substituted stable nitrile oxides
AUTHOR(S): Grundmann, Christoph; Richter, Reinhard
CORPORATE SOURCE: Mellon Inst., Pittsburgh, PA, USA
SOURCE: Journal of Organic Chemistry (1967), 32(7), 2308-12
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:54096
IT 13012-21-0P 13012-22-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 13012-21-0 CAPLUS
CN Benzamidoxime, 4-(dimethylamino)-2,6-dimethyl-N-phenyl- (8CI) (CA INDEX NAME)



RN 13012-22-1 CAPLUS

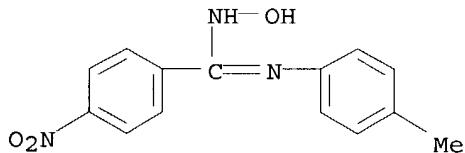
CN Isophthalamidoxime, 4-(dimethylamino)-2,6-dimethyl-N,N'-diphenyl- (8CI) (CA INDEX NAME)



AB cf. CA 66: 37812e. Nitrile oxides of the benzene and pyrimidine series, stabilized by controlled steric hindrance and substituted by a Me_2N group,

are described and some of their reactions discussed. These compds. are the 1st isolated nitrile oxides which contain an addnl. different functional group. 21 references.

L3 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1965:431660 CAPLUS
 DOCUMENT NUMBER: 63:31660
 ORIGINAL REFERENCE NO.: 63:5630f-h, 5631a-b
 TITLE: Synthesis of 2-oxo-1,2,3,5-oxathiadiazoles
 AUTHOR(S): Eloy, F.; Lenaers, R.
 CORPORATE SOURCE: Union Carbide European Res. Assoc., Brussels
 SOURCE: Bulletin des Societes Chimiques Belges (1965), 74 (3-4), 129-35
 CODEN: BSCBAG; ISSN: 0037-9646
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 IT 2630-07-1, p-Benzotoluidide, 4-nitro-, oxime
 (preparation of)
 RN 2630-07-1 CAPLUS
 CN Benzenecarboximidamide, N-hydroxy-N'-(4-methylphenyl)-4-nitro- (9CI) (CA
 INDEX NAME)

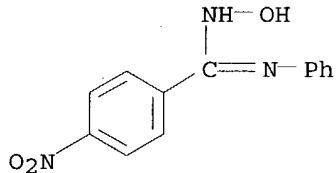


GI For diagram(s), see printed CA Issue.
 AB A series of derivs. (I) of 2-oxo-1,2,3,5-oxathiadiazole was prepared by the dipolar addition of sulfinylamines to nitrile oxides. I were also formed by treating the appropriate N-substituted amide oxime with SOCl_2 in $\text{C}_5\text{H}_5\text{N}$. $\text{p-C}_6\text{H}_4(\text{CNO})_2$ (3.2 g.) in 100 cc. dioxane stirred .apprx.12 hrs. with 5.6 g. PhNSO (II) yielded 7.6 g. III, m. 180° (decomposition). $\text{p-O}_2\text{NC}_6\text{H}_4\text{CCl}:\text{NOH}$ (IV) (10 g.) in the min. amount EtOH treated dropwise at -10 to -5° with 6 g. Et_3N gave 7.8 g. $\text{p-O}_2\text{NC}_6\text{H}_4\text{CNO}$ (V), m. 95°. V (3.3 g.) and 2.8 g. II added at 10° to 100 cc. dry C_6H_6 and the mixture kept 2 hrs. at room temperature and refluxed 0.5 hr. yielded 6 g. I ($\text{R} = \text{p-O}_2\text{NC}_6\text{H}_4$, $\text{R}1 = \text{Ph}$) (VI), m. 140° (C_6H_6 -hexane). IV (10 g.) and 6.9 g. II in 150 cc. dry C_6H_6 treated with 5 g. Et_3N and kept at room temperature overnight gave 4 g. VI, m. 140° . V (1.64 g.) in 50 cc. dry C_6H_6 treated dropwise with 1.19 g. BuNSO in C_6H_6 and kept overnight yielded 0.250 g. I ($\text{R} = \text{p-O}_2\text{NC}_6\text{H}_4$, $\text{R}1 = \text{Bu}$), m. 54° (petr. ether). IV (20 g.) in 100 cc. dry Et_2O treated with 21.4 g. $\text{p-MeC}_6\text{H}_4\text{NH}_2$ in Et_2O and the mixture kept overnight gave 15.5 g. $\text{p-O}_2\text{NC}_6\text{H}_4\text{C}(:\text{NOH})\text{NHC}_6\text{H}_4\text{Me-p}$ (VII), m. 186° (aqueous EtOH). VII (7.8 g.) in 100 cc. dry C_6H_6 containing 6 cc. $\text{C}_5\text{H}_5\text{N}$ treated dropwise at 10° with 3.4 g. SOCl_2 and the mixture kept 2 hrs. and heated 1 hr. at 80° gave 9.5 g. I ($\text{R} = \text{p-O}_2\text{NC}_6\text{H}_4$, $\text{R}1 = \text{p-MeC}_6\text{H}_4$), m. 120° (C_6H_6 -hexane). PrNO_2 (26.7 g.) in 1500 cc. dry C_6H_6 , 72 g. PhNCO , and 42 g. II treated dropwise at 15° with 3 cc. Et_3N in 20 cc. dry C_6H_6 and the mixture kept 3 hrs. at room temperature, heated 3 hrs. at 70° , and refrigerated overnight gave 35 g. I ($\text{R} = \text{Et}$, $\text{R}1 = \text{Ph}$), m. 78° (hexane). Similarly were prepared I ($\text{R} = \text{Et}$, $\text{R}1 = \text{p-MeC}_6\text{H}_4$), I ($\text{R} = \text{Et}$, $\text{R}1 = \text{p-ClC}_6\text{H}_4$), and I ($\text{R} = \text{Et}$, $\text{R}1 = \text{p-MeOC}_6\text{H}_4$) as oils which could not be

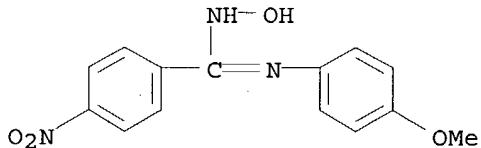
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obtained pure.

L3 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:38478 CAPLUS
DOCUMENT NUMBER: 56:38478
ORIGINAL REFERENCE NO.: 56:7304c-h
TITLE: Decarboxylation of 1,2,4-oxadiazol-5-ones. Syntheses
of benzimidazoles. II
AUTHOR(S): Bacchetti, Tullio; Alemagna, Andreina
CORPORATE SOURCE: Univ. Milan
SOURCE: Atti Accad. Nazl. Lincei, Rend., Classe Sci. Fis.,
Mat. e Nat. (1960), 28, 824-35
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 57767-04-1, Benzanilide, 4-nitro-, oxime 96633-78-2,
p-Benzenoisidide, 4-nitro-, oxime
(preparation of)
RN 57767-04-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX
NAME)

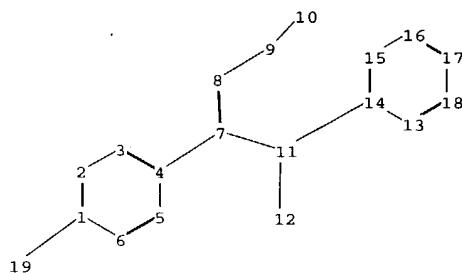
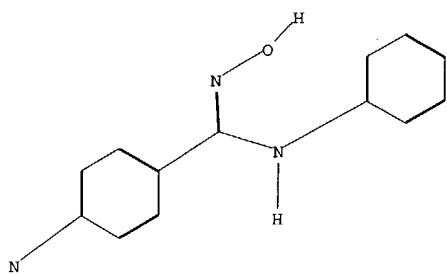


RN 96633-78-2 CAPLUS
CN p-Benzenoisidide, 4-nitro-, oxime (7CI) (CA INDEX NAME)



AB cf. CA 52, 15511g; 55, 16527a. Substituted benzanilide oximes, ArC(:NOH)NHAr', were prepared in 4 ways (A: ArCSNAr' + NH₂OH; B: ArCN → O + Ar'NH₂; C: ArCCl:NOH + Ar'NH₂; D: ArCCl:NAr' + NH₂OH) and converted with ClCO₂Et to oxadiazolones. These were decarboxylated by pyrolysis to give in most cases the corresponding benzimidazoles. The following oximes, oxadiazolones, and benzimidazoles were prepared (Ar and Ar', method of preparation, % yield and m.p. of the benzanilide oxime, % yield and m.p. of the corresponding 1,2,4-oxadiazol-5-one, temperature of pyrolysis, and the % yield, name, and m.p. of the product given): Ph, o-MeC₆H₄, D, -, 86, 148°, 220°, 91.5, 2-phenyl-4methylbenzimidazole (246°); Ph, o-O₂NC₆H₄, D, -, 86, 125°, 255°, 78, 2-phenyl-4-nitrobenzimidazole (I), -; Ph, m-O₂NC₆H₄, D, 60, 127°, 80, 142°, 190°, 93, I, 194° (40%) [and 2-phenyl-5-nitrobenzimidazole (II), m. 203° (60%)]; Ph, p-O₂NC₆H₄, D, -, 152°, 85, 125°, 230°, 75, II, 203°; p-O₂NC₆H₄, Ph, D, 65, 183°, 90, 201°, 220°, 73.5,

2-(p-nitrophenyl)benzimidazole, 310°; p-MeOC₆H₄, Ph, D, 45, 120-1°, 90, 160°, 190°, 14, 2-(p-methoxyphenyl)benzimidazole. 227°; p-MeOC₆H₄, m-O₂NC₆H₄, D, -, 135°, 75, 173°, 190°, 28, 2-(p-methoxyphenyl)-4-(and 5)-nitrobenzimidazole, 228-33°; Ph, β-naphthyl, D, 80, 182°, 91, 181°, 220°, 71, 2-phenyl-α(or β)-naphthimidazole (III), -. Ph, α-naphthyl, B, 90, 177°, 89, 141°, 250°, 26.5, III, -. p-O₂NC₆H₄, p-MeOC₆H₄, D, 70, 163°, 88, 172°, 220°, -, -, -; Ph, p-EtOC₆H₄, B, 65, 157°, 88, 138°, 250°, -, -, -; Ph, β-pyridyl, A, -, 188°, 50, 168°, 180°, -, -, -. Two bis(oxadiazolones) were obtained. Oxanilide dioxime refluxed 12 hrs. in dioxane (IV) with ClCO₂Et, the precipitate washed with H₂O and crystallized from IV yielded 3,3'-bis(4-phenyl-1,2,4-oxadiazol-5-one), m. 265°. Preparation by method C gave 71% oxalo-p-toluidide dioxime (V), m. 201°. V treated in IV with ClCO₂Et gave 68% 3,3'-bis(4-p-tolyl-1,2,4-oxadiazol-5-one) m. 261°. Benzanilide oxime (VI) rearranged with PCl₅ in Et₂O to PhNHCONHPh. Pyrolysis of VI at 165-200° yielded a small amount of 2-phenylbenzimidazole.



chain nodes :

7 8 9 10 11 12 19

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18

chain bonds :

1-19 4-7 7-8 7-11 8-9 9-10 11-12 11-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-19 7-8 7-11 8-9 11-14

exact bonds :

4-7 9-10 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

isolated ring systems :

containing 1 : 13 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS